Theor Chem Acc (1998) 99:420–425
DOI 10.1007/s002149800m30

Theoretical
Chemistry Accounts

Regular article

Efficient boundary basis functions for time-independent quantum scattering calculations

Hyo Weon Jang*

Department of Chemistry, Sunchon National University, Sunchon, Chonnam, 540-742, South Korea

Received: 17 June 1998 / Accepted: 13 July 1998 / Published online: 18 September 1998

Abstract. Novel parametrically energy-dependent boundary functions, F, combined with a finite L^2 basis set, permit accurate and efficient calculation of scattering wavefunctions for many energies. Both accuracy and efficiency are achieved simultaneously because all the necessary integrals are energy-independent and also certain functionals, $(H-E)|F\rangle$, in the Schrödinger equation are allowed to satisfy desirable boundary conditions. In addition, slight modification of the Schrödinger equation in the boundary region is shown to be useful for improving the numerical accuracy when a cutoff-radius-truncated basis set is used. The advantages of the present approaches are demonstrated for the one-dimensional Eckart barrier problem.

Key words: Quantum scattering calculation method

1 Introduction

It is often necessary to use exact quantum mechanical approaches if the most detailed information regarding the scattering process of microscopic particles is required [1]. A class of such approaches is composed of several methods for solving the time-independent Schrödinger equation (SE) in a numerically exact manner, in which the scattering wavefunctions are calculated either explicitly (such as in the approaches of Jang and Light [2], Mandelshtam and Taylor [3], and Kouri et al. [4]) or implicitly (such as in the various Kohn variational methods for K matrix [5], R matrix [6], T matrix and scattering matrix of Miller and coworkers [7,8], and log-derivative matrix of Manolopoulos et al. [9]). The scattering wavefunctions in these methods may be represented by linear combinations of a finite basis set. Since the outcome of scattering is physically determined inside some finite interaction region, all the above approaches can produce exact scattering results in the limit of infinite size of the basis set, at least in principle, if properly used.

The basis sets commonly used are composed of the usual real L^2 functions vanishing at the boundaries. In addition, it is also necessary to include auxiliary basis functions which do not vanish at the boundary located in the direction of dissociation for the scattering wavefunctions involved to be truthful solutions throughout the defined region. These functions must vanish at the other boundaries to yield regular scattering wavefunctions. For convenience, we call such functions boundary functions to emphasize their nonvanishing behavior at the appropriate boundaries. Further classification of these methods can be made according to (1) whether the scattering wavefunctions are defined in an infinite range or only in a finite range; (2) whether the boundary functions are scattering energy-independent or energy-dependent; (3) whether the integrals of the matrix elements are energy-independent or energy-dependent; (4) whether the integrals are real or complex quantities. Such characteristics may affect the performance of a particular approach, such as the rate of convergence to exact results or the amount of computation to achieve a given accuracy.

In this work we deal exclusively with truthful representations of scattering wavefunctions in a finite range (we choose the L^2 basis function to vanish at the boundaries of the finite region). In this particular case, the boundary functions can be chosen as energy-independent and real functions. This choice enables all integrals to be real quantities and reusable for scattering calculations at other energies, which is a useful feature in studying resonances, e.g., [2, 9]. In spite of such formally advantageous features, the calculated wavefunctions are sometimes not uniformly accurate in the defined range (see below for details). For example, when the basis functions are not capable of representing arbitrary functions near the boundary, the accuracy decreases there [10]. This behavior was observed when a truncated basis set (whose zeroth-order energies are below the chosen cutoff values) and/or the particle-in-a-box eigenfunctions (or equivalents) are used [10]. To avoid such undesirable influences, scattering information was

* Supported by the Nondirected Research Fund, Sunchon National University

extracted somewhat inside the range [10], or energy-dependent boundary functions were used in previous studies [11]. Unfortunately, in the latter case, the notorious Kohn anomaly may occur at some scattering energies at which real energy-dependent boundary functions become linearly dependent on the other real L^2 basis functions [12].

After narrowing down the cause of such inaccuracy to the unfavorable boundary conditions of certain functionals involved in the calculation, we develop a novel form of boundary function in this work. It allows the scattering wavefunction to be much more uniformly accurate and the integrals to be energy-independent and real. Also, the numerical results are guaranteed to be free of the Kohn anomaly.

In a somewhat nonrelated context, the degradation of wavefunction accuracy close to the boundary is also observed when a truncated basis set, trimmed from a primitive basis set according to a cutoff radius criterion, is used (i.e., when only the basis functions acting near the interaction region are kept for the subsequent calculation). Such truncation is often desirable when studying generic reactive scattering, in which the coordinate system for basis set definition cannot be superimposed on the natural scattering and internal motion coordinates (e.g., Jacobi coordinates).

In this work, we improve the accuracy of the wavefunction, by forcing the component of the scattering wavefunction expanded by the L^2 basis set to vanish smoothly toward the basis set boundary. This may be done by modifying the regular SE near the boundary in a prescribed way. It turns out that the solution to this modified SE is still truthful and more accurate than otherwise in the inner region where no modification is applied (see below).

2 Theory

We detail the theory of the present two novel approaches below. For simplicity of presentation, we consider one-dimensional scattering with one channel open; the generalization for higher dimensional problems should be straightforward.

In the finite range scattering wavefunction (FRSW) method [2], the linearly independent solutions of the SE in a finite range are determined by solving appropriate matrix-vector equations. Then, the scattering wavefunctions satisfying asymptotic boundary conditions (e.g., the unit-flux incoming wave boundary conditions) are determined by matching the solutions to the known asymptotic behavior. Mathematically, the matching procedure is equivalent to setting up a system of linear equations for unknown scattering matrix elements and expansion coefficients of the solutions, and subsequently, solving for the unknowns.

A particular linearly independent solution ψ of the SE in a finite range $[a,b]$ is represented by a boundary function, F and real L^2 basis functions $\{V_i\}$ as follows.

$$\psi = F + \chi = F + \sum_i C_i V_i \tag{1}$$

where F satisfies the so-called $(0,1)$ and V_i satisfies $(0,0)$ boundary conditions in the range $[a,b]$ (i.e., $F(a)=0$, $F(b)=1$, and $V_i(a)=V_i(b)=0$) [9]. The range $[a,b]$ is chosen to encompass the interaction and minimal asymptotic regions (here, we assume the regions around both a and b are in the asymptotic regions). The expansion coefficients C_i are determined such that Eq. (1) could give the approximate solution of the SE, $(H-E)|\psi\rangle = 0$, where H is the system Hamiltonian operator and E is the scattering energy

$$V_j|H-E|\psi\rangle = \langle V_j|H-E|F\rangle + \sum_i \langle V_j|H-E|V_i\rangle C_i = 0 \ . \tag{2}$$

2.1 Novel boundary function

Note that if F in Eq. (2) is chosen to behave asymptotically as the regular solution ϕ of the unperturbed SE, i.e., $(H_0-E)|\phi\rangle = 0$ where $H_0 = H-U$ and U is the interaction potential, $(H-E)|F\rangle$ vanishes asymptotically. It is observed that such a scattering energy-dependent boundary function yields more uniformly accurate ψ than a fixed energy-independent F could do in general cases (see below for an example). The disadvantage of this energy-dependent F is that the integrals $\langle V_j|H-E|F\rangle$ have to be recalculated for each different choice of scattering energy E and the results may be subject to the Kohn anomaly if it is chosen as a real function. The cause of the Kohn anomaly is given elsewhere [12].

In this work, we consider a particular form of F, which is given by $f_1 + E\cdot f_2$ where f_1 and f_2 are energy-independent fixed real boundary functions. In particular, we determine f_1 and f_2 by requiring that $(H-E)|f_1 + E\cdot f_2\rangle$ vanishes at both boundaries a and b. The practical procedure for finding f_1 and f_2 is given below where H_0 is just kinetic energy operator. Let F be a quartic polynomial with the expansion coefficients determined to satisfy the desired boundary conditions,

$$F(R) = pR + qR^2 + uR^3 + vR^4 \tag{3}$$

such that

$$(H-E)|F\rangle = 0 \text{ at } R=a,\ R=b \quad \text{and } F(a)=0,\ F(b)=1 \tag{4}$$

where p,q,u,v are some constants for a particular choice of $[a,b]$. F, obtained by solving the system of linear equations implied by Eqs. (3) and (4), is given by

$$F(y) = f_1(y) + E\cdot f_2(y) \tag{5}$$

$$f_1(y) = \frac{1}{2}y + \frac{3}{5}y^2 - \frac{1}{10}y^4$$

$$f_2(y) = \frac{m(b-a)^2}{2\hbar^2}\left(\frac{1}{12}y + \frac{1}{20}y^2 - \frac{1}{12}y^3 - \frac{1}{20}y^4\right)$$

where y is related to the scattering coordinate R by a scaling factor y where $y = \frac{(2R-b-a)}{(b-a)}$ and m is the system reduced mass. All the related integrals are real and energy-independent ($\langle V_i|H|f_1\rangle$, $\langle V_i|H|f_2\rangle$, $\langle V_i|f_1\rangle$, and $\langle V_i|f_2\rangle$). The matrix elements involving F in Eq. (2) are

simply constructed by their combinations with the scattering energy E or its square as multiplicative factors in an obvious manner. Note that the functions derived in Eq. (5) are universal and also usable for other systems. This choice of boundary function yields a much more uniformly accurate ψ, which is automatically free of the Kohn anomaly . These points will be demonstrated by test calculations below.

The reason behind this better performance may be understood by noting that $(H-E)|F\rangle$ satisfies $(0,0)$ boundary conditions unlike in the case of arbitrary boundary functions. This has the following consequences. Often, the basis set with $(0,0)$ boundary conditions used to expand χ of Eq. (1) is composed of the eigenfunctions of the asymptotic Hamiltonian H_0. Then, $(H-E)|\chi\rangle$ obviously has the same $(0,0)$ boundary conditions. In this case, since $(H-E)|\psi\rangle$ can be written as $(H-E)|F\rangle+(H-E)|\chi\rangle$, the fact that $(H-E)|F\rangle$ satisfies the same $(0,0)$ boundary conditions helps $(H-E)|\psi\rangle$ to satisfy $(0,0)$ boundary conditions more easily than otherwise. Therefore, the equality implied by the SE can be easily achieved numerically. In addition, since all parts composing the integrand in Eq. (2) satisfy the same $(0,0)$ boundary conditions of the Gaussian quadratures based on $\{V_i\}$, the integrals should be evaluated more accurately as a sum of quadratures than otherwise.

2.2 Basis truncation

When a reactive scattering problem is studied, the range of the $(0,0)$ boundary condition basis set (which is often a direct product of basis functions in several dimensions) must encompass the interaction plus some asymptotic regions. By doing so, some extra regions, covered by the basis set, are inevitably included. For example, these may be the classically forbidden region for the scattering energy considered, or the asymptotic region not needed for scattering information extraction. They are not necessary for the subsequent scattering wavefunction calculation.

A common method to avoid such waste is to simply discard the basis functions corresponding to the extra regions. This is particularly simple to do for a point-wise basis set like the discrete variable representation (DVR) basis [13,14], and we restrict ourselves to this kind of representation. The subsequent calculation produced somewhat accurate results in the past [3,15]. However, in the present work, a close investigation of the wavefunction behavior in a one-dimensional case reveals that the truncated basis set results are less accurate than otherwise. The results obtained using all the primitive basis functions are much more accurate, even when the number of basis functions and ranges are about the same in both cases (see below).

Before discussing the cause behind this observation, it may be helpful to distinguish two different types of truncation, i.e., by a potential energy criterion and by a cutoff radius criterion. The truncation warranted by the former criterion should cause essentially no complication. The scattering wavefunction vanishes smoothly into the classically forbidden region for physical reasons, so it should cause no numerical error if the basis functions located in that region are not included in the calculation from the beginning. To describe the scattering wavefunction accurately we only need to ensure that the boundary function F also vanishes in this region. In other words, it is known that the corresponding expansion coefficients would be essentially zero if the discarded functions were included before any numerical calculations were made. In passing, we note that ignoring a particular basis function is equivalent to setting the corresponding coefficients to zero in terms of the full primitive basis set representation.

On the other hand, the portion of the wavefunction which would be expanded by the basis functions discarded by a cutoff-radius criterion does not necessarily vanish for any physical reason. Effectively, it is equivalent to setting the coefficients to zero rather abruptly for those discarded functions which are located beyond the cutoff radius in terms of the full primitive basis set representation. This may result in nonphysical discontinuities in the scattering wavefunction and/or its derivatives being responsible for the inaccurate results.

To avoid such abrupt change in the solution, we modify the SE near the cutoff radius (which is now the boundary of the truncated basis set) so that we arbitrarily force χ to vanish smoothly toward (and beyond) the boundary as follows;

$$(1-g)(H-E)|F+\chi\rangle+g|\chi\rangle=0 \tag{6}$$

where g is a kind of cutoff function which is zero for most of the basis set range and increases slightly toward the

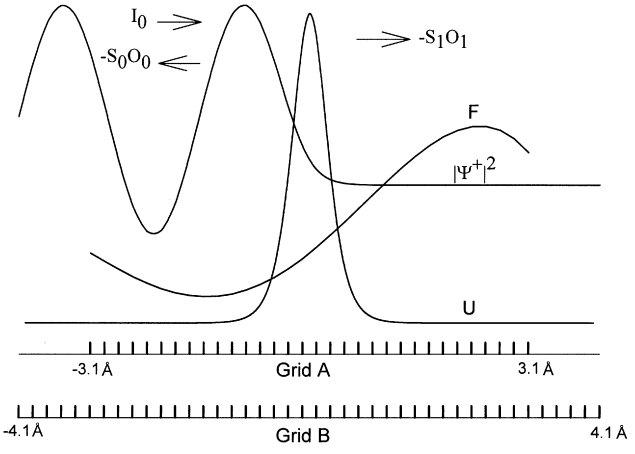

Fig. 1. Schematic representation of the Eckart barrier problem. The parameters of the Hamiltonian operator are chosen as $m = 4.3$ g/mol, $\alpha = 3.0\text{Å}^{-1}$, $D = 10\,\text{cm}^{-1}$. The Eckart barrier is denoted by U, the magnitude squared of the scattering wavefunction at $E = 6\,\text{cm}^{-1}$ by $|\Psi^+|^2$ and a sample boundary function (Eq. 5) by F which increases from zero to unity on *Grid A* passing from left to right. The asymptotic boundary conditions are denoted by "$I_0 - S_0O_0$" and "$-S_1O_1$" in the reactant and product regions, respectively, where the subscripts $0,1$ denote the reactant and product waves and I, O denote the incoming and outgoing waves, respectively, while S_0, S_1 are scattering matrix elements determining the reflection and transmission probabilities, respectively. *Grid A* corresponds to the full basis set used for Fig. 2 and *Grid B* defines the primitive basis set, from which the truncated basis set used for Fig. 3 is obtained. Both grids are spaced by 0.2 Å

outer boundary b. In this way, the scattering wavefunction $F+\chi$ transforms smoothly into F toward the boundary, while the aforementioned unfavorable discontinuities are alleviated. Note that this modification corresponds to forcing the expansion coefficients implied in χ to vanish smoothly toward the boundary in a pointwise representation such as DVR. As long as we extract the scattering information where the solution is truthful (i.e., away from the boundaries), the results should be more accurate than otherwise (see below for an example).

3 Compartive calculation and discussion

We combine the present novel boundary functions with the FRSW method [2] to calculate the transmission probabilities of an incoming particle through a one-dimensional Eckart barrier [16]. The Hamiltonian operator and wavefunctions are represented by the DVR based on the particle-in-a-box eigenfunctions and also all integrals involved are evaluated by the Gaussian quadratures based on the same eigenfunctions. The SE equation to be solved is

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dR^2}+\frac{D}{\cos h^2(\alpha R)}\right]\psi = E\psi \tag{7}$$

where the system parameters are given in the legend to Fig. 1.

A schematic representation of the barrier, a sample novel boundary function, the magnitude squared of a sample scattering wavefunction, and the grids of DVR used for actual calculations are presented in Fig.1. In the present application of the FRSW method, two linearly independent solutions of the SE are obtained first by solving Eq. (2) adopting two boundary functions of the form of Eq. (5) (these are mirror images through the peak of the barrier). Then, the scattering wavefunction Ψ^+, which satisfies the unit-flux incoming wave boundary condition, is obtained by matching the linear combination of the above two solutions to the appropriate asymptotic boundary conditions. The actual location of matching is at R_1, R_2 on the product side asymptotic region (matched to $-S_1O_1$), and at R_3, R_4 on the reactant side asymptotic region (matched to $I_0 - S_0O_0$), respectively, as follows:

$$\Psi^+(R_i) = A\Psi(R_i) + B\Psi(R_i) = -S_1\sqrt{\frac{m}{k}}\exp(ikR_i), \tag{8}$$

$$\Psi^+(R_j) = A\Psi(R_j) + B\Psi(R_j) = \sqrt{\frac{m}{k}}\exp(ikR_j) - S_0\sqrt{\frac{m}{k}}\exp(-ikR_j)$$

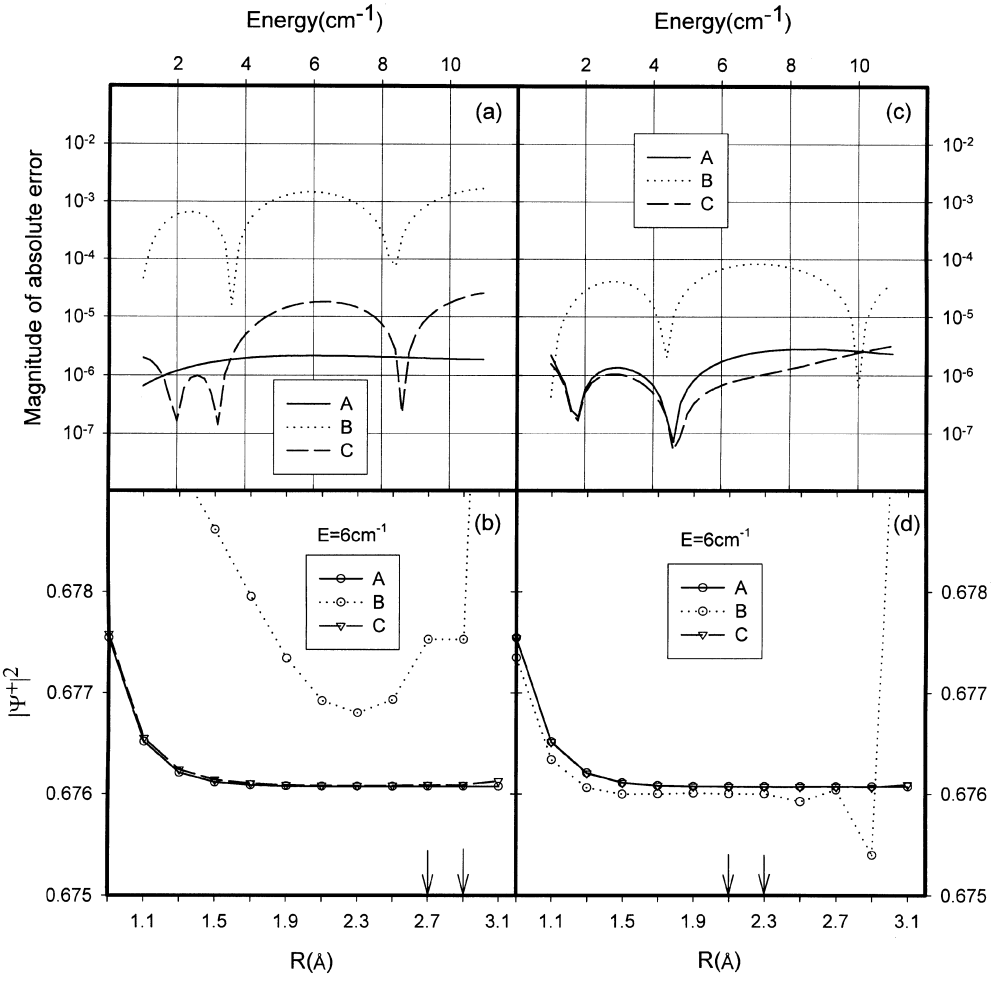

Fig. 2a–d. Comparisons of numerical results obtained by the previous and present approaches. **a** and **c** show the magnitude of absolute errors in the energy range $[1\,\mathrm{cm}^{-1}, 11\,\mathrm{cm}^{-1}]$ and **b** and **d** show the magnitude squared of scattering wavefunctions along the coordinate at the scattering energy $6\,\mathrm{cm}^{-1}$. *A* denotes the results of using the real solutions of the unperturbed SE, *B* is of the fixed linear functions, and *C* is of the present novel functions, for boundary functions, respectively. The two plots of the left column (i.e., **a** and **b**) use coordinates of ±2.9 Å and ±2.7 Å for matching and those of the right column (i.e., **c** and **d**) use ±2.3 Å and ±2.1 Å. The basis set is composed of 30 DVR basis functions in the range $[-3.1\,\text{Å}, 3.1\,\text{Å}]$ (see Fig. 1)

where R_i and R_j are the centers of the appropriate DVR basis functions in each asymptotic region, respectively, and k is the wavenumber of a chosen scattering energy E. The transmission probability is given as $|S_1|^2$, obtained from solving the appropriate system of linear equations for the unknown constants, A, B, S_0, and S_1.

In Figs. 2 and 3 we compare the magnitude of absolute errors in numerical results against the analytically exact transmission probabilities [16] for three different choices of boundary function: (A) real solutions of the unperturbed SE (i.e., $\sin(kr)$ and $\cos(kr)$); (B) fixed linear functions; (C) parametrically energy-dependent boundary functions [see Eq. (5)], among which the last is new. For the energies considered here ($[1\text{cm}^{-1}, 11\text{cm}^{-1}]$), the transmission probabilities vary from ~ 0.18 to ~ 0.85 as the scattering energy increases. Also, the squares of the magnitudes of the scattering wavefunctions are plotted along the scattering coordinate in the product asymptotic region at the scattering energy of $6\,\text{cm}^{-1}$, which is in the middle of the energy range considered. The magnitude in the product asymptotic region should be identical to the transmission probability, so it must be essentially constant, in an accurate calculation.

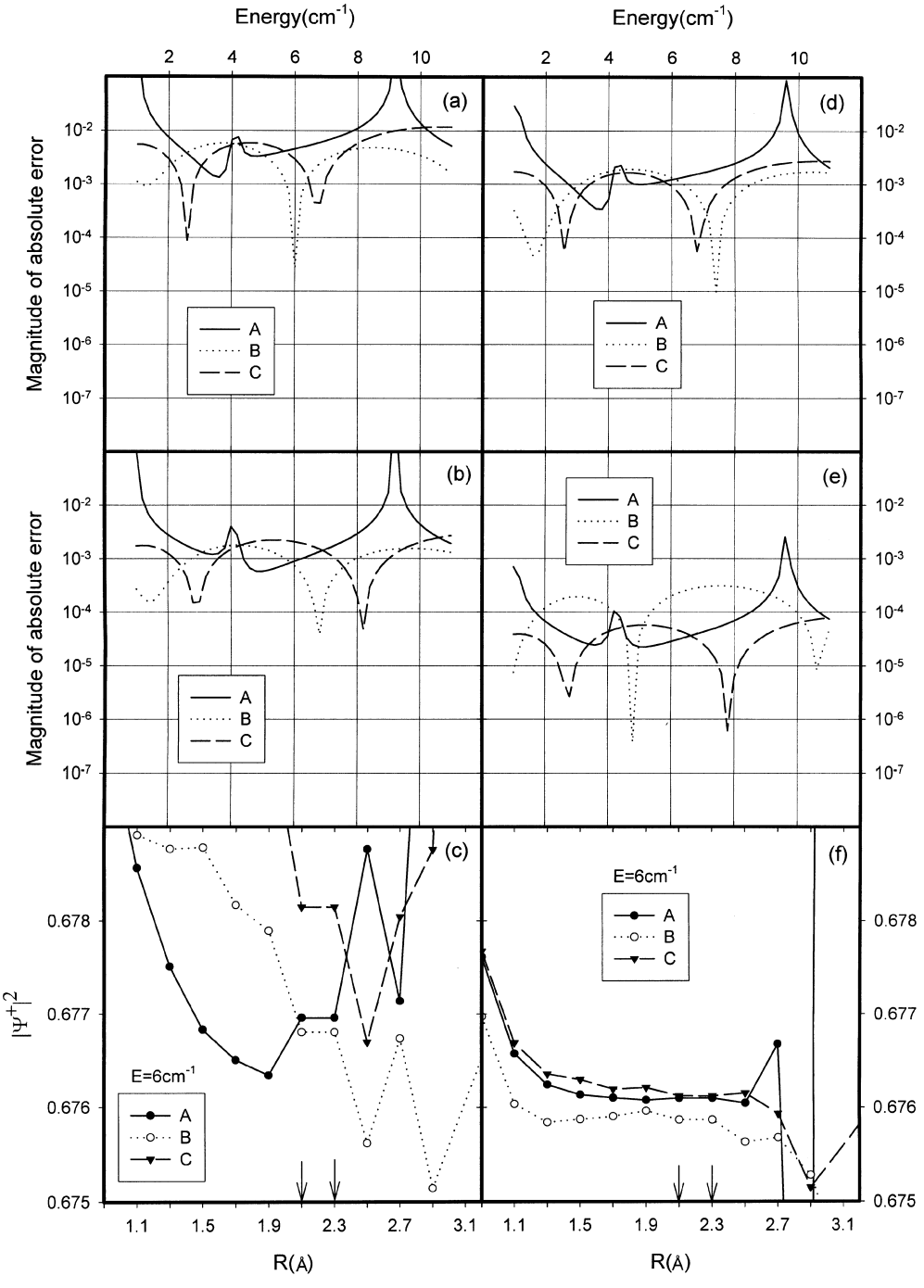

Fig. 3a–f. Comparisons of numerical results obtained by the previous and present approaches when a truncated basis set is used. **a**, **b**, **d**, and **e** show the magnitude of absolute errors in the energy range $[1\,\text{cm}^{-1}, 11\,\text{cm}^{-1}]$ and **c** and **f** show the magnitude squared of scattering wavefunctions along the coordinate at the scattering energy of $6\,\text{cm}^{-1}$. A denotes the results of using the real solutions of the unperturbed SE, B is of the fixed linear functions, and C is of the present novel functions, for boundary functions, respectively. The three plots of the left column (i.e. **a**, **b**, and **c**) denote the results for no modification of the SE and those of the right column (i.e., **d**, **e**, and **f**) denote the results for the present modification of the SE. The g function in Eq.(6), used for SE modification, is adjusted to be 0.00033535 at ± 2.9 Å and zero elsewhere for the best results. The two plots on the top row (i.e., a and d) use the coordinates ± 2.7 Å and ± 2.5 Å for matching and the remaining plots use ± 2.3 Å and ± 2.1 Å. The truncated basis set is composed of 30 DVR basis functions in the range $[-3.0$ Å$, 3.0$ Å$]$ obtained from the 40 primitive functions in the range $[-4.1$ Å$, 4.1$ Å$]$ (see Fig.1)

3.1 Test for novel boundary function

An examination of the absolute errors in the transmission probabilities of Fig. 2 reveals that the least accurate results are for (B) among the three cases, although the errors are less than 0.001 for most of the energies. The most accurate results are for (A) or (C), depending on the matching locations. If the matching is done closest to the boundary, (A) of the previous approach gives better accuracy (Fig. 2a), but if matched somewhat inside the range, (C) of the present approach is better than (A) (Fig. 2c). For both (B) and (C), the accuracy improves by about an order of magnitude if matching is done somewhat inside the range than if done at the outermost points, while there is no significant improvement for (A) (cf Fig. 2a and 2c).

These trends in relative magnitude of errors are also reflected in the behavior of the squares of the magnitudes of the scattering wavefunctions. They become almost constant in the asymptotic region for (A) and (C), but not so for (B), although (A) appears slightly better than (C) (Fig. 2b and 2d).

These observations suggest that the use of the present novel boundary functions is definitely better than that of the fixed linear function, but may not be significantly better than the use of previous energy-dependent boundary functions in terms of the relative uniformity of wavefunctions. However, we emphasize that the amount of numerical computation is essentially the same and relatively small for both (B) and (C) if calculations are done for many energies while (A) requires recalculation of $\langle V_i|H-E|F\rangle$ for each energy. Besides, there is a danger of a Kohn anomaly in the results for (A) which does not occur in this particular calculation (see below for an opposite example).

3.2 Test for modified SE for truncated basis set

Next, we consider the results of using a truncated basis set. We retain part of the primitive DVR basis functions whose centers are located inside a cutoff radius from the peak of the barrier for the subsequent scattering calculations (Fig. 1). In Fig. 3 we compare the results of the regular brute force truncation calculations with those done by applying the modification of Eq. (6). Though the size and range of the basis set is about the same as for Fig. 2 calculations which use all the primitive basis functions, the absolute errors are generally larger in this case. However, the present approach of SE modification clearly improves the accuracy for (A), (B), and (C), by up to an order of magnitude for most of the energies (cf. Fig. 3a and 3d, Fig. 3b and 3e). There are no clear differences in accuracy among the three cases without modification (Fig. 3a–c), but modification introduces greater improvement for (A) and (C) than for (B) (Fig. 3d-f). This is even more obvious if the matching is done somewhat inside (cf. Fig. 3a and 3d, Fig. 3b and 3e).

The peaks in the error curves in case (A) are a consequence of a Kohn anomaly. Either of the two energy-dependent boundary functions ($\sin(kr)$ or $\cos(kr)$) appears to vanish at the boundaries of the symmetric range around the energies of the peaks ($\sim 1\ \mathrm{cm}^{-1}$, $\sim 4.5\ \mathrm{cm}^{-1}$, and $\sim 9.5\ \mathrm{cm}^{-1}$). Therefore, even if the results are more accurate in case (A) for some of the energies, it may be best to use (C) for general purposes because of the better stability in accuracy and greater savings in the amount of computation (The dips denote that the sign of errors are changing).

The magnitude squared of scattering wavefunctions behavior clearly shows how much the present modification of the SE improves the accuracy of the results for all types of boundary functions tested, especially if matching is done somewhat inside the range (cf. Fig. 3c and 3f).

4 Concluding remarks

The present novel boundary functions allow all the integrals to be energy-independent and real while maintaining about the same level of accuracy as provided by the more computationally demanding energy-dependent-integral approaches. Also, the present modification of the SE may allow the size of matrix involved to be greatly reduced for multidimensional scattering problems while achieving more improved accuracy than no modification provides. The two novel approaches presented in this work are expected to be most useful for reactive scattering problems in more than one-dimensional mathematical space where the efficiency and accuracy implied by a particular algorithm would essentially determine whether the actual calculation is doable or not.

Acknowledgement. The author acknowledges the financial support of the Nondirected research fund, Sunchon National University, for the year 1997–1998.

References

1. Levine RD, Bernstein RB (1987) Molecular reaction dynamics and chemical reactivity. Oxford University Press, New York
2. Jang HW, Light JC J Chem Phys (1993) 99: 1057
3. Mandelshtam VA, Taylor HS J Chem Phys (1995) 102: 7390
4. Kouri DJ, Arnold M, Hoffman DK Chem Phys Lett (1993) 203: 166
5. Nesbet RK (1980) Variational methods in electron-atom scattering theory. Plenum, New York
6. Burke PG, Robb WD (1975) In: Bates DR, Robb WD (eds) Advances in atomic and molecular physics, vol 11. Academic Press, New York, p 144
7. Miller WH, Jansen op de Haar BMDD (1987) J Chem Phys 86: 6213
8. Zhang JZH, Chu S-I, Miller WH (1988) J Chem Phys 88: 6233
9. Manolopoulos DE, Wyatt RE (1988) Chem Phys Lett 152: 23
10. Jang HW, Choi SE, Light JC (1994) J Chem Phys 100: 4188
11. Manolopoulos DE, D'Mello M, Wyatt RE (1990) J Chem Phys 93: 403
12. Jang HW, Light JC (1996) Mol Phys 89: 111
13. Light JC, Whitnell RM, Park TJ, Choi SE (1989) In: Lagana A (ed) NATO ASI series C vol 277 Reidel, Dordrecht, p 187
14. Colbert DT, Miller WH (1992) J Chem Phys 96: 1982
15. Jang HW, Light JC (1995) Chem Phys Lett 242: 62
16. Landau LD, Lifshitz EM (1977) Quantum mechanics, 3rd edn. Pergamon Press, Oxford